Class 7: Fluorite, pyrochlore, murataite

- $z = \frac{3}{4}$
  - fcc
  - rock salt

- $z = \frac{1}{2}$
  - diamond
  - zinc blende

- $z = \frac{1}{4}$
  - Fm-3m

- $z = 0$
  - Fd-3m
  - F-43m
  - Fm-3m

Materials 286 G: Structural Families of Functional Inorganic Materials
Ram Seshadri x6129 seshadri@mrl
Class 7: Fluorite, pyrochlore, murataite

Views of the fluorite CaF$_2$ structure [Gerlach 1922]. Ca is 8-coordinate and F is 4-coordinate. Many oxides: UO$_2$, PrO$_2$, CeO$_2$, stabilized, cubic ZrO$_2$ and HfO$_2$...

Uses: CeO$_2$ is an oxide ion conductor. HfO$_2$ and ZrO$_2$ are important structural materials. UO$_2$ is “yellowcake”
Class 7: Fluorite, pyrochlore, murataite

Stabilized zirconia:

- cubic
- mono baddeleyite
- tet

stabilization with $Y_2O_3$
Class 7: Fluorite, pyrochlore, murataite

H. G. Scott,
Phase relationships in the zirconia-yttria system
JOURNAL OF MATERIALS SCIENCE 10 (1975) 1527-1535

Fluorite oxides are highly radiation tolerant because they are able to accommodate point defects easily: *Science* **289** (2000) 748.
Class 7: Fluorite, pyrochlore, murataite

Fluorite

8 coordination + 8 coordination

\[ \text{A}_2\text{B}_2\text{O}_8 \rightarrow \text{A}_2\text{B}_2\text{O}_7 \]

Pyrochlore

8 coordination + 6 coordination
Class 7: Fluorite, pyrochlore, murataite

Pyrochlore views:

- $A_2B_2O_6O'$
- $B_2O_6$
- $A_2O'$

Stellated *Kagomé* lattice of $B_4$ tetrahedra. The central atom is $O'$. This is a motif found in spinel as well.
A wide variety of pyrochlore structures are known: A can be Ca, Cd, Tl, Pb, Bi, Ln etc. B can be transition metals as well as main group elements. The A and B sites can be mixed. O' can be absent, or can be F−, OH− etc.

Pyrochlores can be insulating, metallic, magnetic ...


Class 7: Fluorite, pyrochlore, murataite

Murataites:


The fluorite is a 3D chessboard of regular cubes. The pyrochlore has one half of the cubes replaced by octahedra, and one eighths of the anions missing. The pyrochlore can be constructed by making the coloring the fluorite chessboard. This is a 2x2x2 ordering.

More complex 3x3x3 ordering gives the murataite.